Magneto-thermal evidence of a partial gap at the Fermi surface of UPt_2Si_2

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Motivated by the observation of a giant Nernst effect in URu_2Si_2, the thermoelectric response of the related system UPt_2Si_2 was investigated using thermal and electric transport properties such as the Nernst and Seebeck effects, thermal conductivity, Hall effect and electrical resitivity. Unlike URu_2Si_2, UPt_2Si_2 is neither superconducting nor exhibits a "hidden-order" state. Nevertheless a pronounced Nernst effect anomaly is found to coincide with the onset of the antiferromagnetic order in UPt_2Si_2. Although the absolute values are substantially lower, its appearance and characteristics can favorably be compared to the giant Nernst effect in URu_2Si_2 indicating the common feature of a partial Fermi surface gap.

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The mysterious nature of the "hidden-order" (HO) phase in URu_2Si_2, discovered more than 20 years ago, is still unresolved [1, 2, 3]. Initially HO was associated with a weak antiferromagnetic order setting in at $T_{HO} \simeq 17.5\,\mathrm{K}$ [4, 5], however recent experiments have shown this transition to be essentially non-magnetic [6]. Transport properties such as the Seebeck effect or the Nernst and Hall effects are very sensitive in detecting slight changes in the charge carrier spectrum at the Fermi energy. The appearance of a giant Nernst effect [7] emerging with the onset of the HO impelled the investigation of these transport properties in the related system UPt_2Si_2 which forms a local-moment antiferromagnetic ground state [8].

While for the high-temperature superconductors [9, 10, 11] the anomalous part of the Nernst effect is caused by moving flux lines, other mechanisms have to be held responsible for systems comprising the various classes of heavy fermions [7, 12, 13], semimetals [14], ferromagnetic metals [15, 16, 17] or organic compounds [18, 19]. Among these are anomalous scattering mechanisms like "side jump" [20] or "skew scattering" [21]. They are driven by magnetic order and are sources to the anomalous components of the Hall effect. Furthermore in some systems Nernst effects can arise due to a combination of unusual physical properties. According to Oganesyan and Usshishkin [22], a large Nernst signal can arise in systems that combine lightweight charge carriers, long scattering lifetimes and reduced Fermi energies. Not only the latter but also a gap or a partial gapping of the Fermi surface (FS) has been identified as the source of anomalies in the Nernst effect [23] and the thermoelectric power [24] in antiferromagnets. These calculations consider the presence of a superzone gap in addition to phonon and spin scattering mechanisms.

In this Letter, we present thermal and electric transport properties such as the Nernst and Seebeck effects, thermal conductivity, Hall effect and electrical resitivity. The predictions that arise from the calculations of [23, 24] include substantial changes in the Nernst, Seebeck and Hall effects with their interrelated scaling and a maximum formation at about $0.5 \cdot T_N$. All these features are in very good agreement with the measurements presented here, indicating that gap formation strongly influence these transport properties. However, the considered gapping of the FS can affect only parts of it because the resistivity shows no sign of a metal to insulator transition. Since such a partial gapping has also been observed for URu_2Si_2 at the onset of the HO [25, 26], the appearance of the giant Nernst effect might as well be discussed as being caused by a Fermi surface reconstruction. Our measurements clearly demonstrate that the appearance of a Nernst signal tracks the phase transition at $T_N \simeq 32\,\mathrm{K}$ and its behavior is qualitatively comparable to the effects reported for the HO transition of URu_2Si_2.

The structure of UPt_2Si_2 is tetragonal with lattice constants $a = 4.186\,\mathrm{Å}$ and $c = 9.630\,\mathrm{Å}$. The lattice is of $CaBe_2Ge_2$ type (space group $P4/nmm$). UPt_2Si_2 possesses an antiferromagnetic ground state with $T_N \simeq 32\,\mathrm{K}$ [27]. Neutron diffraction studies revealed magnetic moments of $2.5\,\mu_B$ oriented along the c direction with ferromagnetic coupling within the $a-a$ planes and antiferromagnetic coupling on adjacent planes along the c axis.

The thermal and electric transport measurements have been carried out on two annealed samples of UPt_2Si_2. The as-cast samples were annealed for approximately one week at a temperature of $T = 900°\mathrm{C}$. One sample was oriented such that the application of either a temperature gradient or a transport current was along the a axis with the magnetic field applied along the c axis and the other sample with the transport quantities applied along c which leaves the magnetic field and the transverse components in the $a-a$ plane. Temperature gradients have been applied using a chip heater glued to the top of the sample and were picked up by AuFe-Chromel thermocouples. The setup in which a considerable Nernst signal, $e_N = E_y/(-\nabla_x T)$, could be detected was oriented such that $\nabla T \parallel a$ and $H \parallel c$. In $\nabla T \parallel c$ and $H \parallel a$, no Nernst signal could be resolved so that we will continue focussing upon the former configuration. Figure 1 (lower panel) shows the temperature dependence of the resistivity of UPt_2Si_2 along the a axis with the magnetic field applied along the c axis. Coming from high temperatures

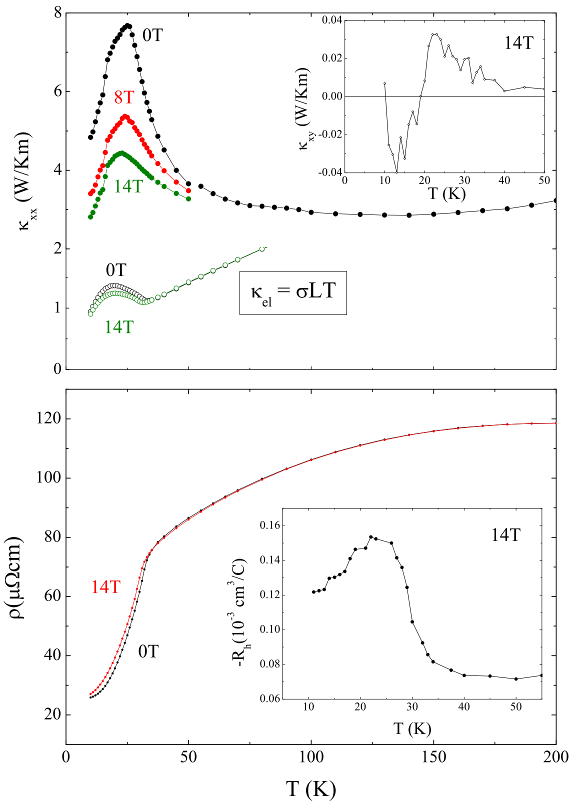

FIG. 1: (Color online) Upper panel: thermal conductivity along the a axis of UPt_2Si_2 for magnetic fields applied along c. The inset shows the off-diagonal component κ_{xy}, which is of the order of 1% of κ_{xx}. The open symbols give an upper-limit estimation of the electronic contribution to the thermal conductivity as calculated by the Wiedemann-Franz law. Lower panel: Resistivity along the a axis in 0 and 14 T along c. The inset shows the temperature dependence of the Hall coefficient of UPt_2Si_2 in 14 T with its pronouced increase below T_N.

$\rho(T)$ shows a very weak temperature dependence with a broad maximum of $\rho(T) \approx 120\mu\Omega$cm around 200 K. At $T_N \simeq 31.5$ K (determined from the maximum of $d\rho/dT$) the transition into the antiferromagnetic phase shows up as a kink in ρ with no signature of a superzone gap. The knee-like reduction of $\rho(T)$ can be modeled within a scenario in which magnetic excitations freeze out due to the opening of a spin-wave gap with $\Delta \approx 44$ K [8, 28]. Electronic transport shows localized behavior along the c axis which near T_N exhibits a clear dip in $d\rho/dT$ denoting the opening of a superzone gap in the charge channel (see Fig. 8 of Ref [8]).

The upper panel of Fig. 1 displays the temperature dependence of the thermal conductivity in zero field, 8 T, and 14 T. For $H = 0$, $\kappa(T)$ demonstrates a weak temperature dependence at high temperatures, with a shallow minimum at $T \approx 125$ K. With decreasing temperature, $\kappa(T)$ develops a peak at about 25 K. The height of the peak is strongly H-dependent, while its position changes with H only very weakly. The inset of the upper panel of Fig. 1 displays the off-diagonal component of the thermal conductivity, κ_{xy}, also referred to as Righi-Leduc effect. The absolute values of κ_{xy} are more than two orders of magnitude smaller than the corresponding κ_{xx} values. The open symbols of Fig. 1 present an estimation of the upper limit of the electronic thermal conductivity $\kappa_{\rm el}$ calculated from the experimental data of $\rho(T)$ using the Wiedemann-Franz law, $\kappa_{\rm el} = LT/\rho$ with $L = 2.45{\cdot}10^{-8}\,{\rm W}/\Omega{\rm K}^2$ being the Lorenz number. At low T, the calculated $\kappa_{\rm el}$ is much smaller than the total measured κ; besides, it does not account for the strong suppression of κ by magnetic field. This indicates that the thermal conductivity in UPt_2Si_2 is predominantly phononic. The strong sensitivity of thermal conductivity to the magnetic field in a broad temperature region, both above and below T_N, suggests that spin fluctuations play an important role as scatterers of phonons. It is surprising, however, that no clear anomaly of $\kappa(T)$ is observed at the magnetic ordering transition, see e.g.[29].

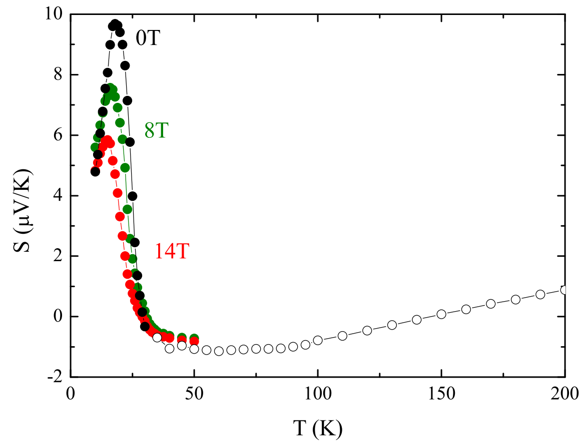

FIG. 2: (Color online) Thermopower of UPt_2Si_2 for magnetic fields of 0, 8 T, and 14 T ($\nabla T||a$, $H||c$).

The onset of the antiferromagnetic ordering is also accompanied with an enhancement of the thermopower (Fig. 2) which furthermore becomes field dependent such that increasing fields suppress $S(T,H)$. The zero-field thermopower exhibits a steep increase in the vicinity of the antiferromagnetic order and peaks at about half T_N. Applying a magnetic field leads to a gradual suppression of the absolute values of $S(T \leq T_N)$ and slightly shifts its maximum to lower T.

A large Nernst signal emerges below the antiferromagnetic transition temperature of $T_N \simeq 32$ K as depicted in Fig. 3. The signal is not anomalous in a way that it deviates from a field-linear quasiparticle background as is the case in many high-temperature superconductors. The signal here just rises below the temperature of antiferromagnetic order and displays a linear field dependence. Upon lowering the temperature, e_N gradually increases until a maximum at ≈ 15 K is reached. Further cooling causes a decrease of the signal.

In order to fully analyze the various contributions that

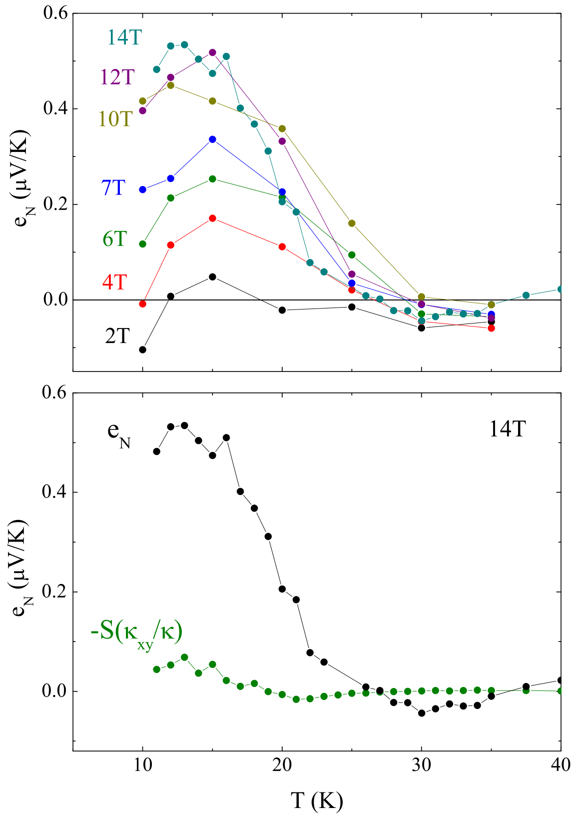

FIG. 3: (Color online) Upper panel: Temperature dependence of the Nernst signal of UPt_2Si_2 in various magnetic fields. Lower panel: Comparison of the temperature dependent thermal Hall contribution to the measured Nernst signal, in $H = 14\,\mathrm{T}$ ($\nabla T || a$, $H || c$).

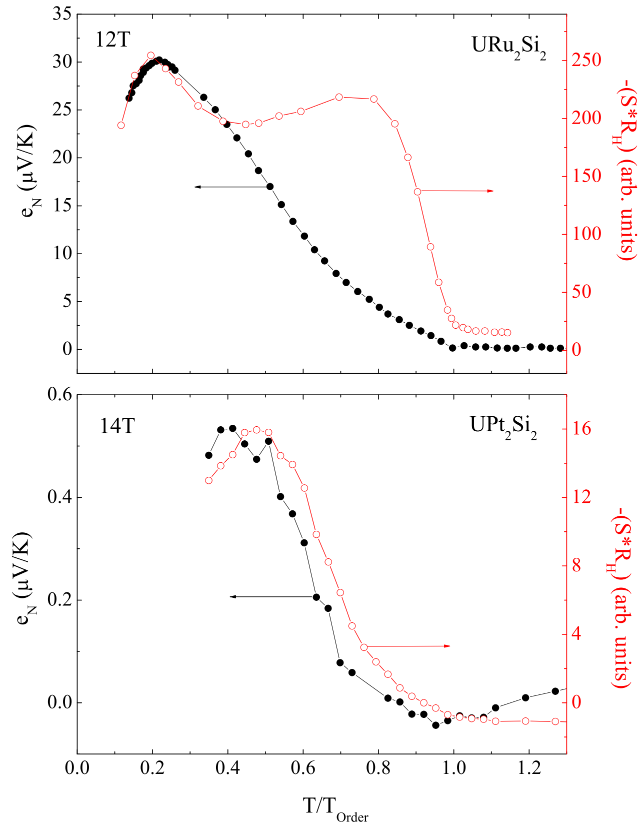

FIG. 4: (Color online) Upper panel: The Nernst signal of URu_2Si_2 compared to the product of its thermopower and Hall coefficient at $H = 12\,\mathrm{T}$. Data are taken from [7] with a $T_{Order} = T_{HO} = 17.5\,\mathrm{K}$. The lower panel depicts the scaling behavior for UPt_2Si_2 as expected from calculations for a generic antiferromagnet due to the opening of a superzone gap [23]. The maximum positions of roughly $0.5{\cdot}T_{Order}$ well agree with the theoretical expectations. Here, $T_{Order} = T_N = 31.5\,\mathrm{K}$.

the adiabatic Nernst signal may be composed of [13], the Seebeck effect, Hall effect and Righi-Leduc effect have been additionally measured as already introduced,

$$e_N = \rho\alpha_{xy} - S\left[\frac{\sigma_{xy}}{\sigma} + \frac{\kappa_{xy}}{\kappa}\right]. \qquad (1)$$

Here, α and $\sigma = \rho^{-1}$ denote the Peltier and conductivity tensor, respectively. To detect tiny transverse temperature gradients, an AuFe-Chromel thermocouple has been attached directly to the wires that pick up transverse voltages. The difference between the isothermal and the adiabatic Nernst signal is given by the product of the thermopower and κ_{xy}/κ and is shown in Fig. 3 (lower panel) at 14 T. It becomes clear that the magnitude of the thermopower that might add to the transverse voltages due to a transverse temperature gradient is much smaller than the measured e_N. In 14 T, κ_{xy}/κ_{xx} is of the order of 1% so that its product with the thermopower $S(T, 14\mathrm{T})$ results in a contribution of less than 10% of the measured $e_N(T, B)$. Thus, we can safely discuss the Nernst signal as being essentially isothermal.

Using a free-electron relaxation time model, Abelskii *et al.* [23, 24] have calculated the Nernst and Seebeck effects for generic ferro- and antiferromagnetic materials. The antiferromagnets possess a superzone gap due to the doubling of the lattice periodicity. This charge gap when combined with spin and phonon scattering causes a large contribution to the Nernst and Seebeck signals below T_N while the resistivity shows a much smaller effect. The calculations predict a maximum of the thermopower between 0.4 to $0.6{\cdot}T_N$ [24]. The Nernst coefficient is calculated in a similar manner, and is found to display also a maximum at about half T_N [23]. Within these calculations the Hall coefficient is also subjected to a steep increase after crossing into the antiferromagnetic phase. A further prediction of the calculation is a scaling of the Nernst effect with the product of the thermopower and the Hall coefficient [23].

Let us compare these predictions with our measurements, starting with the thermopower in Fig. 2. The characteristic of $S(T)$ clearly displays the calculated features, a steep increase below T_N with the maximum value appearing at about half T_N. The Nernst effect, shown in Fig. 3 also is in very good agreement with its calculated prognoses: a pronounced increase just below T_N together

with the maximum formation around $0.5 \cdot T_N$. In addition, the Hall coefficient meets the predicted behavior [23] as well. As shown in Fig. 4 (lower panel), the theory is once again nicely verified with respect to the scaling behavior, since the experimental data clearly display the proportionality $e_N \propto (S \cdot R_H)$.

Figure 4 (upper panel) displays such a scaling for the related system URu_2Si_2 ($T_{HO} = 17.5\,\mathrm{K}$), where it becomes evident that the underlying physics of both substances cannot be completely of the same origin. The scaling is vastly disturbed between $0.4{\cdot}T_{HO}$ and T_{HO}. The differences between these two systems are obviously caused by the complicated behavior of the thermopower in that temperature region [7]. Furthermore the positions of the maxima at $\approx 0.2 \cdot T_{HO}$ of e_N and S are shifted to lower values than the expected $0.5{\cdot}T_{Order}$. One may speculate here that the HO phase is responsible for additional features besides those calculated for a generic antiferromagnet [23, 24]. Nevertheless, the Nernst signal of UPt_2Si_2 shown in Fig. 3 qualitatively resembles the Nernst signal found in URu_2Si_2 ($e_{N,max}(12\,\mathrm{T}) \approx 30\,\mu\mathrm{V/K}$) where it develops just below the HO ordering temperature [7], although it is much lower in absolute values ($e_{N,max}(12\,\mathrm{T}) \approx 0.5\,\mu\mathrm{V/K}$).

In summary, we found the emergence of a large Nernst signal in UPt_2Si_2 below T_N, which is accompanied by anomalies in the thermopower and the Hall coefficient. These features very well agree to predictions of Refs. [23, 24] for antiferromagnets under the assumption of a gapping of the Fermi surface below T_N. Our transport measurements suggest that the gap evolving in the charge channel has to be attributed to only a portion of the Fermi surface very much like that suggested for URu_2Si_2. These are common features in both related substances, URu_2Si_2 and UPt_2Si_2, but the model used for UPt_2Si_2 is not completely suitable for URu_2Si_2, indicating the influence of the itinerant character of the hidden-order phase. Nevertheless, the behavior of the Nernst effects in both systems may be connected to the gapped regions of the Fermi surface.

Acknowledgments

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[1] T.T.M. Palstra, A.A. Menovsky, J. vandenBerg, A.J. Dirkmaat, P.H. Kes, G.J. Nieuwenhuys, and J.A. Mydosh. Phys. Rev. Lett. **55**, 2727 (1985).

[2] W. Schlabitz, J. Baumann, B. Pollit, U. Rauchschwalbe, H.M. Mayer, U. Ahlheim, and C.D. Bredl. Z. Physik B **62**, 171 (1986).

[3] M.B. Maple, J.W. Chen, Y. Dalichaouch, T. Kohara, C. Rossel, M.S. Torikachvili, M.W. Mc Elfresh, and J.D. Thompson. Phys. Rev. Lett. **56**, 185 (1986).

[4] C. Broholm, H. Lin, P.T. Matthews, T.E. Mason, W.J.L. Buyers, M.F. Collins, A.A. Menovsky, J.A. Mydosh, and J.K. Kjems. Phys. Rev. B **43**, 12809 (1991).

[5] C. Broholm, J.K. Kjems, W.J.L. Buyers, P. Matthews, T.T.M. Palstra, A.A. Menovsky, and J.A. Mydosh. Phys. Rev. Lett. **58**, 1467 (1987).

[6] H. Amitsuka, K. Matsuda, I. Kawasaki, K. Tenya, and M. Yokoyama. J. Magn. Magn. Mat. **310**, 214 (2007).

[7] R. Bel, H. Jin, K. Behnia, J. Flouquet, and P. Lejay. Phys. Rev. B **70**, 220501(R) (2004).

[8] S. Suellow, A. Otop, A. Loose, J. Klenke, O. Prokhnenko, R. Feyerherm, R.W.A. Hendrikx, J.A. Mydosh, and H. Amitsuka. J. Phys. Soc. Jpn. **77**, 024708 (2008).

[9] Z.A. Xu, N.P. Ong, Y. Wang, T. Kakeshita, and S. Uchida. Nature **406**, 486 (2000).

[10] Y. Wang, L. Li, and N.P. Ong. Phys. Rev. B **73**, 024510 (2006).

[11] N. Johannsen, T. Wolf, A.V. Sologubenko, T. Lorenz, A. Freimuth, and J.A. Mydosh. Phys. Rev. B **76**, 020512(R) (2007).

[12] R. Bel, K. Behnia, Y. Nakajima, K. Izawa, Y. Matsuda, H. Shishido, R. Settai, and Y. Onuki. Phys. Rev. Lett. **92**, 217002 (2004).

[13] Y. Onose, L. Li, C. Petrovic, and N.P. Ong. EPL **79**, 17006 (2007).

[14] K. Behnia, M.A. Measson, and Y. Kopelevich. Phys. Rev. Lett. **98**, 076603 (2007).

[15] T. Miyasato, N. Abe, T. Fujii, A. Asamitsu, S. Onoda, Y. Onose, N. Nagaosa, and Y. Tokura. Phys. Rev. Lett. **99**, 086602 (2007).

[16] P.A. Lee. Physica C **408-10**, 5 (2004).

[17] Y. Taguchi, Y. Oohara, H. Yoshizawa, N. Nagaosa, and Y. Tokura. Science **291**, 2573 (2001).

[18] M.S. Nam, A. Ardavan, S.J. Blundell, and J.A. Schlueter. Nature **449**, 584 (2007).

[19] W. Wu, I.J. Lee, and P.M. Chaikin. Phys. Rev. Lett. **91**, 056601 (2003).

[20] L. Berger. Phys. Rev. B **2**, 4559 (1970).

[21] J. Smit. Physica **21**, 877 (1955).

[22] V. Oganesyan and I. Ussishkin. Phys. Rev. B **70**, 054503 (2004).

[23] E.G. Dik and S.S. Abelskii. Soviet Physics - Solid State **17**, 454 (1975).

[24] S.S. Abelskii and Y.P. Irkhin. Soviet Physics - Solid State **13**, 2035 (1972).

[25] J.R. Jeffries, N.P. Butch, B.T. Yukich, and M.B. Maple. Phys. Rev. Lett. **99**, 217207 (2007).

[26] Y.J. Jo, L. Balicas, C. Capan, K. Behnia, P. Lejay, J. Flouquet, J.A. Mydosh, and P. Schlottmann. Phys. Rev. Lett. **98**, 166404 (2007).

[27] R.A. Steeman, E. Frikkee, S.A.M. Mentink, A.A. Menovsky, G.J. Nieuwenhuys, and J.A. Mydosh. J. Phys. – Condens. Matter **2**, 4059 (1990).

[28] N.H. Andersen. *Crystalline Electric Field and Structural Effects in f-electron Systems*. Plenum, New York (1980).

[29] K. Berggold, J. Baier, D. Meier, J.A. Mydosh, T. Lorenz, J. Hemberger, A. Balbashov, N. Aliouane, and D.N. Argyriou. Phys. Rev. B **76**, 094418 (2007).

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